Alternatives Analysis Workshop on Life Cycle Impacts & Exposure Assessment

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University of California, Santa Barbara

August, 2018

ADVANCED TOPICS

Dr. Sangwon Suh (Aug 10th, 1:00pm-1:45pm)

Advanced Topics

- What to do if there is no data? Or if available data points are of poor quality?
  - Data gaps and quality assessment
  - Qualitative and quantitative uncertainty analysis

Advanced Topics

- **Data gaps and quality assessment**
- Qualitative and quantitative uncertainty analysis

9.3 Addressing Data Gaps

- "… the responsible entity may use any of a variety of approaches to **address data gaps.**"

- "help the responsible entity to **identify relevant factors, support decision-making**, and select future research efforts."

From AA Guide p114

Process-specific Data Gaps

- Data gap for a specific process for a particular chemical and product combination (e.g., lack of data on resource and materials consumption and emissions/discharge from the process);
- Inadequate data for a particular region, time period, or technology;

Modified from AA Guide p114

Address Process-specific Data Gaps

- Use **proxy data** sets or **extrapolated data** to provide a reasonable estimate
  - Use existing environmental data from one process to represent a similar process;
  - It is important to consider the data source, accuracy, age, etc;

Modified from AA Guide p115, 116

Proxy Method 1

Method 1: Direct proxy

If product A and product B are assumed to have equivalent function and similar characteristics,

process emissions of product B = process emissions of product A.

From AA Guide p115

Proxy Method 2

Method 2: Averaged proxy

If product A is manufactured in region A and product B is manufactured in country B, and assuming, process emissions of product B = Weighted average process emissions of product A from four countries in Region A according to production volume (C1 represents country 1, C2 is country 2, etc.),

process emissions (PE) of product B = [(% of volume $_{C1}$)(PE_{C1} of product A) + (% of volume $_{C2}$)(PE_{C2} of product A) + (% of volume $_{C3}$)(PE_{C3} of product A) + (% of volume $_{C4}$)(PE_{C4} of product A)]

Proxy Method 3

Method 3: Scaled proxy

For a multi-component product B, if process emissions data are available for 85% weight of the components represented by product A then the data gap is bridged by linearly scaling up the data for 85% of component to 100%,

$$\text{process emissions of product B} = \frac{\text{PE of product A}}{85\%}$$

Hands-on Example

Chemical-specific Data Gaps

- Data gap for evaluation of hazard traits or potential exposures of chemicals;
- Use read-across and trend analysis (e.g. QSAR) to estimate or predict missing endpoints;

Modified from AA Guide p116

Read-across Method

- A technique to predict toxicity information for one chemical by using toxicity information of another chemical based on their structural or functional similarity;
- Require trained experts to group chemicals based on structural similarity, mechanistic or analogue approach;

Modified from AA Guide p116

Chemical Similarity

- The similarity of chemical structural or functional qualities;
- *"Similar compounds have similar properties."*
- Often used in drug design studies by screening large databases containing structures of available chemicals;

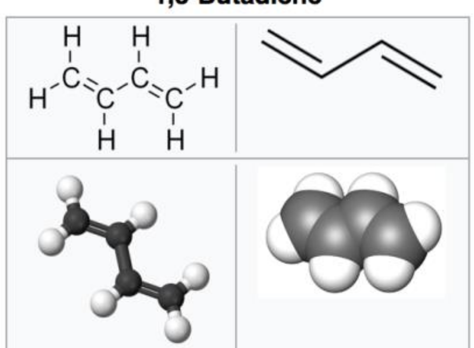
Examples from CLiCC

Using of proxy chemicals

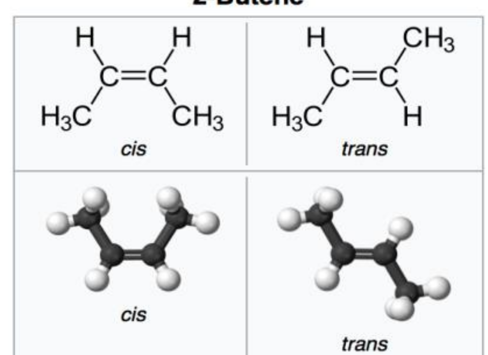
The chemicals listed below are based on structural similarity between butadiene and the chemicals in our database.

Chemical Name	CAS	Similarity
propylene	115-07-1	High
2-butene	107-01-7	High
acrolein	107-02-8	Low

1,3-Butadiene



2-Butene



Trend Analysis

- A technique of predicting toxicology by analyzing **correlations** between a hazard trait to some physicochemical properties;
- e.g. QSAR

Modified from AA Guide p117

QSAR

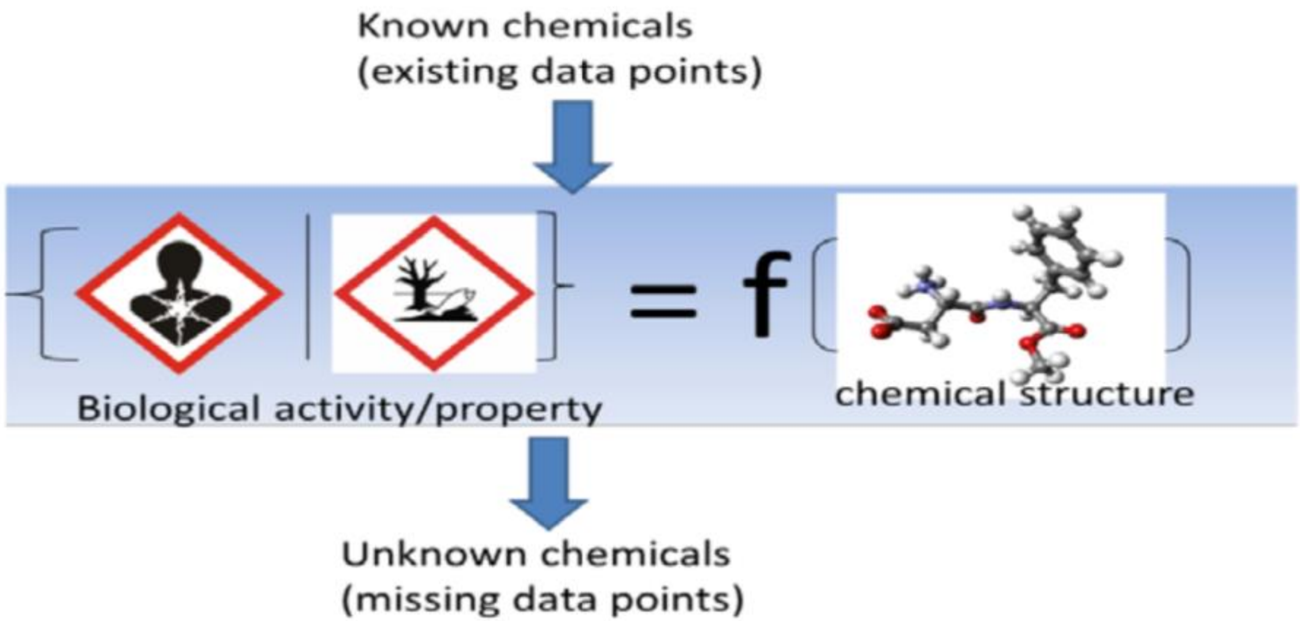


Figure 9-2 Graphical Representation of QSAR Approach to Address Chemical-Specific Data Gaps

From AA Guide p117

CLiCC Example

Human Health Toxicity

	Result	Negative Count	Positive Count	Not Classified Count	Sample Size	Confidence Level	Source
Developmental toxicity (-)	Negative	2	0	0	2	Estimated (Low)	VEGA
Mutagenicity (-)	Negative	2	1	1	4	Estimated (Low)	VEGA
Skin sensitization (-)	Negative	1	0	0	1	Estimated (Low)	VEGA

Ecotoxicity

Ecotoxicity	Mean	Maximum	Minimum	Sample Size	Standard Deviation	Confidence Level	Source
Daphnia magna ChV (mg/L)	6.14E+00	6.14E+00	6.14E+00	1	-	Estimated (Medium)	EPI Suite
Daphnia magna LC50 in 48 hr (mg/L)	2.13E+00	6.29E+01	2.37E-02	3	2.75E+01	Estimated (Medium)	VEGA & EPI Suite
Fathead minnow LC50 in 96hr (mg/L)	7.08E+02	7.08E+02	7.08E+02	1	-	Estimated (Low)	VEGA
Fish Acute LC50 (mg/L)	3.65E+01	3.65E+01	3.65E+01	1	-	Estimated (Low)	VEGA

Address Chemical-specific Data Gaps

- Use measured data from a suitable analog;
- Use approximations based on surrogate data;
- Use estimated data from computational models;

Modified from AA Guide p122

Summary of Data Gap

- Address process-specific and chemical-specific data gaps;
- Document data collection efforts and explain why a chemical is eliminated from consideration due to data gaps;

Modified from AA Guide page 122

Advanced Topics

- Data gaps and quality assessment
- **Qualitative and quantitative uncertainty analysis**

9.4 Addressing Uncertainty

- "…distinguish the **key uncertainties** and **scale of these uncertainties**. The responsible entity may treat uncertainty in several ways."

- "the responsible entity may focus on addressing uncertainties that are likely to have **greater relevance** (i.e., those that prevent them from reaching a reliable AA conclusion)." *(i.e., materiality of uncertainty)*

From AA Guide p123

What is Uncertainty?

- The lack of knowledge
- Random error and statistical variation
- Inherent randomness
- Approximation

Why Does Uncertainty Matter?

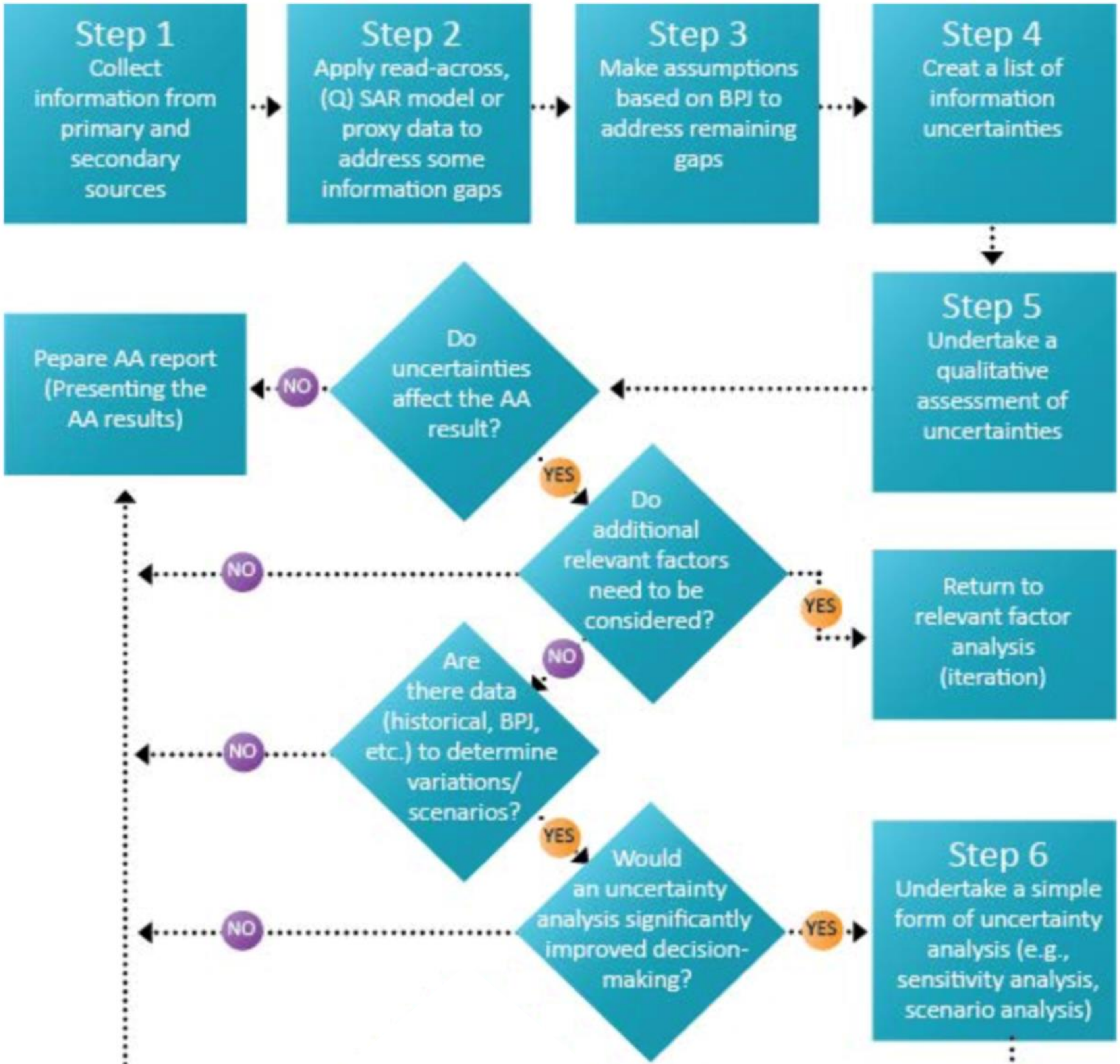
- Uncertainty cannot be completely avoided
- Lead to inaccurate and/or imprecise LCA or RA results
- Uncertainty is useful information
  - Where to focus future research?
  - What are the worst case scenarios?

Sources of Uncertainty

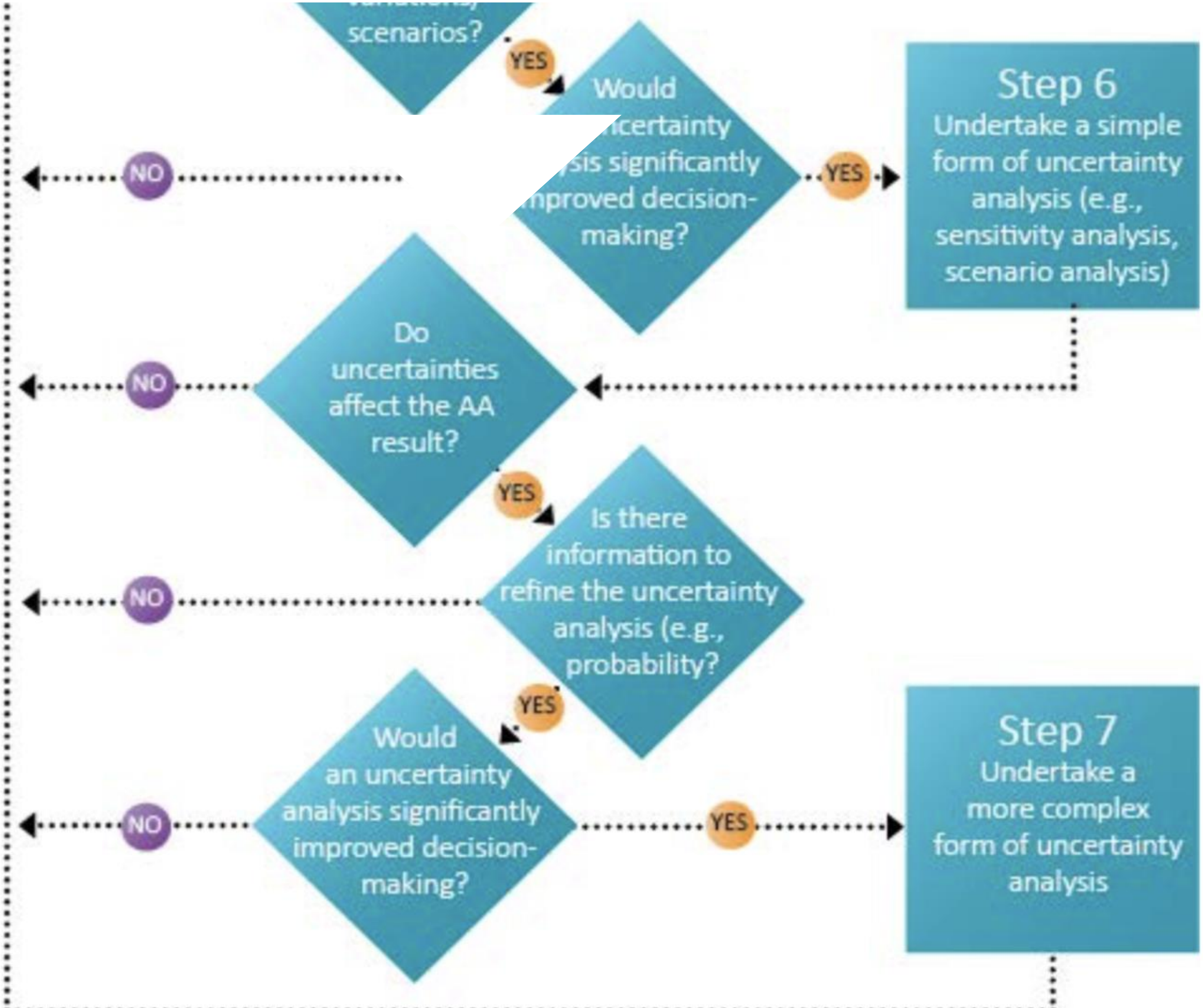
- Parameter uncertainty due to imprecise knowledge of parameters;
- Temporal and spatial variability in parameters;
- Variability between sources in the LCI and between objects of the assessment in the LCIA;
- Uncertainty in the models;
- Uncertainty due to choices in LCA;

Geisler, et al. Uncertainty Analysis in Life Cycle Assessment (LCA): Case Study on Plant-Protection Products and Implications for Decision Making

Recommended Approach to Uncertainty Analysis in A.A. Report (*handout*)



From AA Guide page 124


scenarios?
YES
Would
ncertainty
ysis significantly
nproved decision-
making?
YES
Step 6
Undertake a simple form of uncertainty analysis (e.g., sensitivity analysis, scenario analysis)
NO
Do uncertainties affect the AA result?
NO
YES
Is there information to refine the uncertainty analysis (e.g., probability?
NO
YES
Would an uncertainty analysis significantly improved decision-making?
NO
YES
Step 7
Undertake a more complex form of uncertainty analysis

Step 1: Collect data from primary and secondary sources

- Comprehensive search of the literature and existing databases for available data;
- Scientific literature or measured data from site-specific or process-specific sources;
- High-quality review papers, peer-reviewed advisory reports, published handbooks, or peer-reviewed databases;

Modified from AA Guide p125

Step 2: Apply read-across, QSAR model, or proxy data to address some data gaps

- Use a read-across technique, a trend analysis, or QSAR models for missing chemical-specific information;
- Use proxy data to provide a reasonable estimate;

Step 3: Make assumptions based on best professional judgments to continue AA

- Use expert estimates, historical case reports, or assumptions made based on best professional judgments to address data gap;

Step 4: Create a list of uncertainties

- Identify, consider, and document uncertainties in each step of the AA process;
- Include uncertainties related to approaches to addressing data gaps and assumptions;

Step 5: Undertake a qualitative assessment of uncertainties

- Use available approaches and methods to show the effect and extent of potential uncertainties on their AA outcome;
- For example, a ranking system
  - Use +++, ++, +, -, -- or --- to communicate both the direction (underestimate or overestimate) and magnitude (minor, medium or major effect) of the uncertainties
  - e.g., +++ is a major overestimate; - is a minor underestimate

Assess Data Quality

- Evaluate LCI Data Quality
  - Pedigree Matrix of Data Quality Indicators
  - ISO Standard 14044: Environmental Management – Life Cycle Assessment – Requirements and Guidelines
  - US EPA Guidelines for Assessing the Quality of Life-Cycle Inventory Analysis
- Evaluate Chemical Safety Assessment Data Quality
  - OECD HPV Chemicals Program
  - EU REACH Regulation Guidance Documents
  - IPCS Harmonization Project

Pedigree Matrix of Data Quality Indicators

Indicator Score	1	2	3	4	5 (default)
Reliability	Verified* data based on measure-ments**	Verified data partly based on assumptions or non-verified data based on measurements	Non-verified data partly based on qualified estimates	Qualified estimates (e.g., by industrial expert)	Non-qualified estimate
Completeness	Representative data from all sires relevant for the market considered, over an adequate period to even out normal fluctuations	Representative data from > 50% of the sires relevant for the market consi-dered, over an adequate period to even out normal fluctuations	Representative data from only some sites (<<50%) relevant for the market considered or > 50% of sites but from shorter periods	Representativ e data from only one site relevant for the market considered or some sites but from shorter periods	Representativenes s unknown or data from a small number of sites and from shorter periods
Temporal correlation	Less than 3 years of different to the time period of the dataset	Less than 6 years of different to the time period of the dataset	Less than 10 years of difference to the time period of the dataset	Less than 15 years of difference to the time period of the dataset	Age of data unknown or more than 15 years of difference to the time period of the dataset
Geographical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production conditions	Data from area with slightly similar production conditions	Data from unknown or distinctly different are (North America instead of Middle East, OECD-Europe instead of Russia)
Further technological correlation	Data from enterprises processes and materials under study	Data from processes and material under study (i.e. identical technology) but from different enterprises	Data from processes and materials under study but form different technology	Data on related processes or materials	Data on related processes on laboratory scale or from different technology

Weidema, B.P., Bauer, C., Hischier, R., Mutel, C., Nemecek, T., Reinhard, J., Vadenbo, C. O., and Wernet, G. Overview and Methodology, Data Quality Guideline for Ecoinvent Database Version 3. Ecoinvent Report No. 1 (v3). Swiss Centre for Life Cycle Inventories, St. Gallen, Switzerland, 2013.

An example from US LCI

- Toluene diisocyanate, at plant

Activity | Modeling | Administrative | Exchanges

Name	Toluene diisocyanate, at plant
Category	Chemical Manufacturing - Petrochemical Manufacturing
Description	The toluene diisocyanate data for this module includes data for the production of carbon monoxide, dinitrotoluene (DNT), phosgene, and toluene diamine (TDA). Heat was exported as a coproduct for some producers. The energy amount for the exported heat was reported separately as recovered energy. A large amount of hydrogen chloride is produced as a coproduct during this process. A mass basis was used to partition the credit for each product. This process has net water outputs. The mass imbalance is due to unavailability of the weight of water inputs to production and outputs to nature. The coproduct amount for hydrogen chloride is not shown due to confidentiality issues. Complete inventory data and metadata are available in full in the final report and appendices, Cradle-to-Gate Life Cycle Inventory of Nine Plastic Resins and Four Polyurethane Precursors. This report has been extensively reviewed within Franklin Associates and has undergone partial critical review by ACC Plastics Division members and is available at: www.americanchemistry.com. Quantities may vary slightly between the reference to main source and and this module due to rounding. Important note: although most of the data in the US LCI database has undergone some sort of review, the database as a whole has not yet undergone a formal validation process. Please email comments to lci@nrel.gov.
	North America
Location	RNA (RNA)
Geography Comment	US
Infrastructure Process	False
Quantitative Reference	Toluene diisocyanate, at plant
Start Date	2003-01-01
End Date	2003-01-01
Time description	
Technology Description	Phosgenation of toluene diamine (TDA)

Activity | Modeling | Administrative | Exchanges

Process Type	UNIT_PROCESS
LCI Method	
Modelling constants	
Data completeness	
Data selection	
Data treatment	
Sampling procedure	Data are from primary sources.
Data collection period	
Reviewer	
Other evaluation	
Sources	THE PLASTICS DIVISION OF THE AMERICAN C

Activity | Modeling | Administrative | Exchanges

Flow	Category	Flow Type	Unit	Amount	Comment
Outputs					
Ammonia	water/unspecified	Elementary	kg	2.01e-05	
Ammonia	air/unspecified	Elementary	kg	2.61e-04	
BOD5, Biological Oxygen Demand	water/unspecified	Elementary	kg	4.99e-05	
Benzene, 1,2-dichloro-	air/unspecified	Elementary	kg	1.00e-06	This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.
Benzene, 1,2-dichloro-	water/unspecified	Elementary	kg	1.00e-07	This emission was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.
COD, Chemical Oxygen Demand	water/unspecified	Elementary	kg	1.69e-04	
Carbon dioxide, fossil	air/unspecified	Elementary	kg	6.53e-04	
Carbon monoxide	air/unspecified	Elementary	kg	1.47e-03	
Carbonyl chloride	air/unspecified	Elementary	kg	1.00e-08	This emission (a.k.a. 'phosgene') was reported by fewer than three companies. To indicate known emissions while protecting the confidentiality of individual company responses, the emission is reported only by order of magnitude.

Indicator Score	1	2	3	4	5 (default)
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Pedigree Matrix of Data Quality Indicators

→ ++/--

Weidema, B.P., Bauer, C., Hischier, R., Mutel, C., Nemecek, T., Reinhard, J., Vadenbo, C. O., and Wernet, G. Overview and Methodology, Data Quality Guideline for Ecoinvent Database Version 3. Ecoinvent Report No. 1 (v3). Swiss Centre for Life Cycle Inventories, St. Gallen, Switzerland, 2013.

ISO Standard 14044: Environmental Management – Life Cycle Assessment – Requirements and Guidelines

- Time-related coverage
- Technology coverage
- Completeness
- Representativeness
- Consistency
- Reproducibility
- Sources of the data
- Uncertainty of the information

Modified from AA Guide p214

US EPA Guidelines for Assessing the Quality of Life-Cycle Inventory Analysis

DQI	Relevance of DQI (A)	Data Quality Rating (B)	Comments
Acceptability	High	High	(A) It is important for the data to have undergone review by an independent party. (B) The data received extensive review, including being subject to an extensive QA/QC methodology.
Bias	High	High	(A) Bias in aggregated data can result from over-reliance on data from a new technology, a specific region of the country, or from specific processing method. (B) Data were collected from over 600 mills covering many technologies, processes, and geographic areas. The data were segregated into specific subcategories to avoid overlapping process technologies. Long-term sampling programs were employed which mitigate problems from cyclic variations (e.g., seasonal, business cycle.)
Comparability	High	High	(A) It is important for the data to be comparable to long-term measures of industry effluent. (B) Several test sites were selected for long-term analysis to provide a comparable measure. Data values compared well to these standards.
Completeness	Medium	High	(A) Representativeness is deemed more important than completeness in this analysis. (B) There is considerable data in this data source on the target primary water effluent from 600 mills.

From AA Guide p216

Step 5: Undertake a qualitative assessment of uncertainties

Human health	Model	Input parameter x1	Input parameter x2	Input parameter x3	Scenario
Chemical X	-	+/-	++	+/-	--
Alternative A	+	--	+++	+	+/-
Alternative B	+	+/-	--	+/-	+

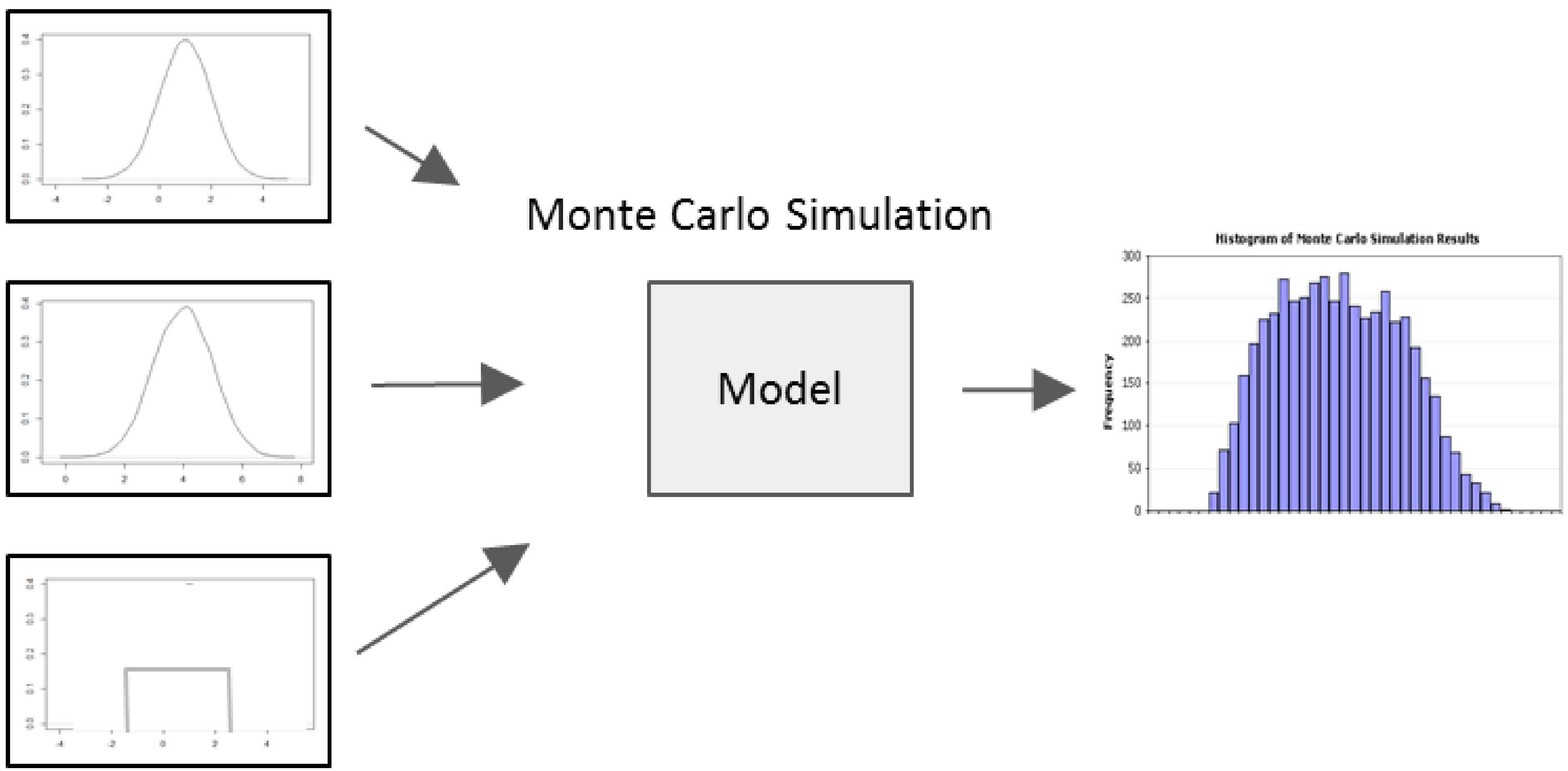
Step 6: Undertake a simple form of quantitative uncertainty analysis

- Use sensitivity analysis or scenario analysis
- Determine the low and high estimates for each major parameter or build worst and best case scenarios
- No further uncertainty analysis is necessary if the AA result is not affected significantly

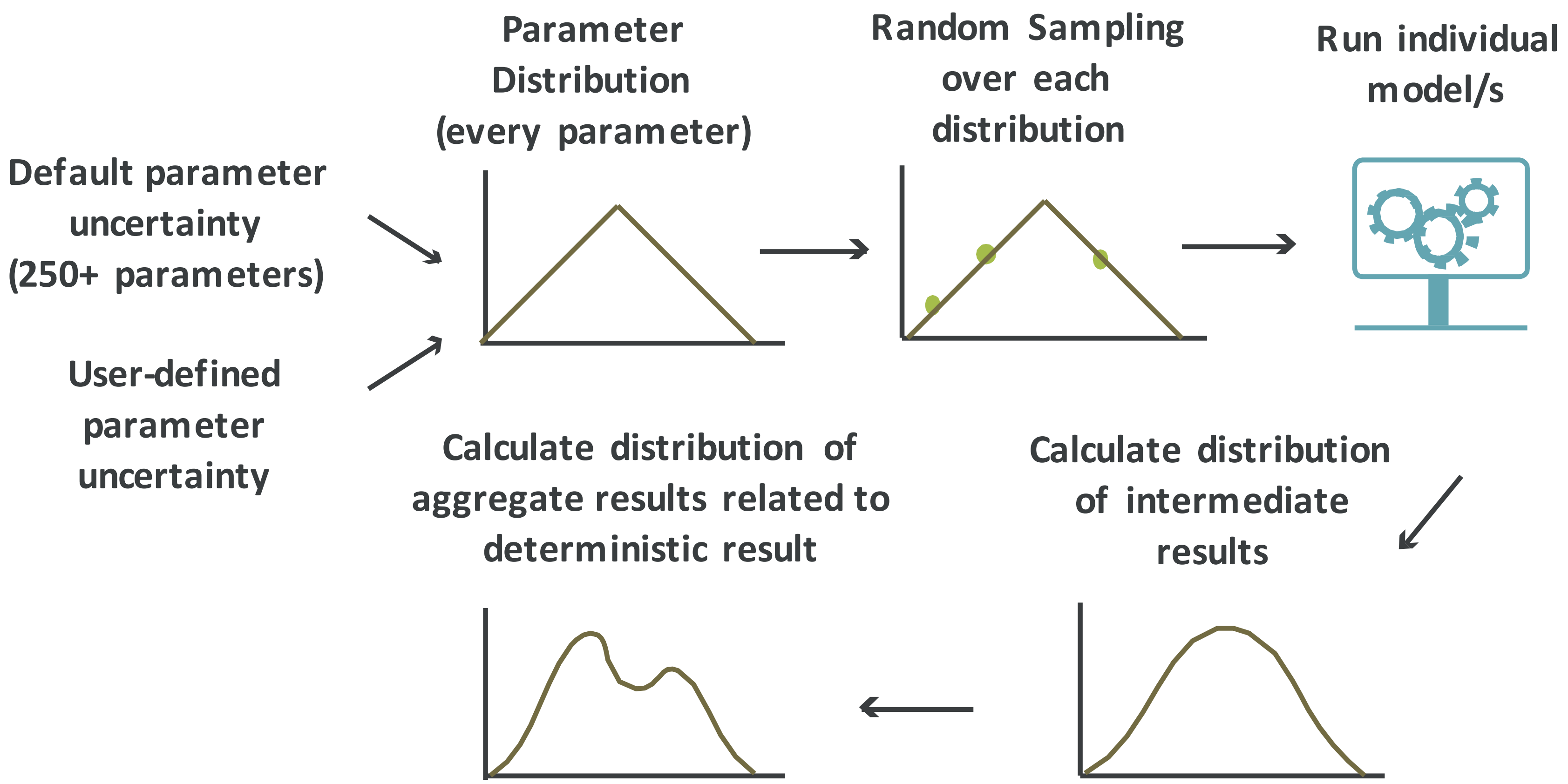
Step 7: Undertake a complex form of uncertainty analysis

- Use statistical methods based on probability distribution to perform uncertainty analysis
- Such as **Monte Carlo simulations**, bootstrapping, fuzzy set theory, and Bayesian analysis

Step 7: Undertake a complex form of uncertainty analysis

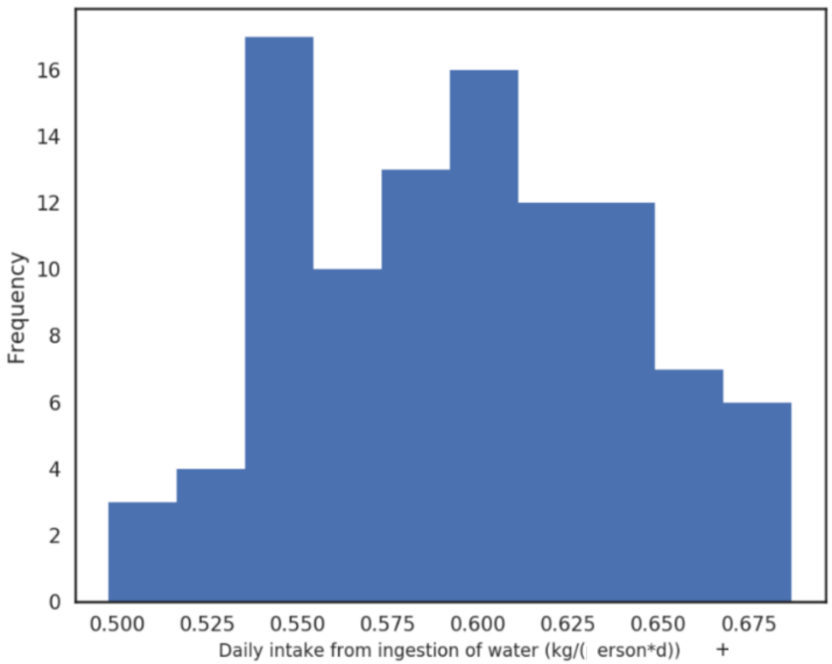


Step 7: Undertake a complex form of uncertainty analysis



Examples from CLiCC

▾ Daily intake from ingestion of water



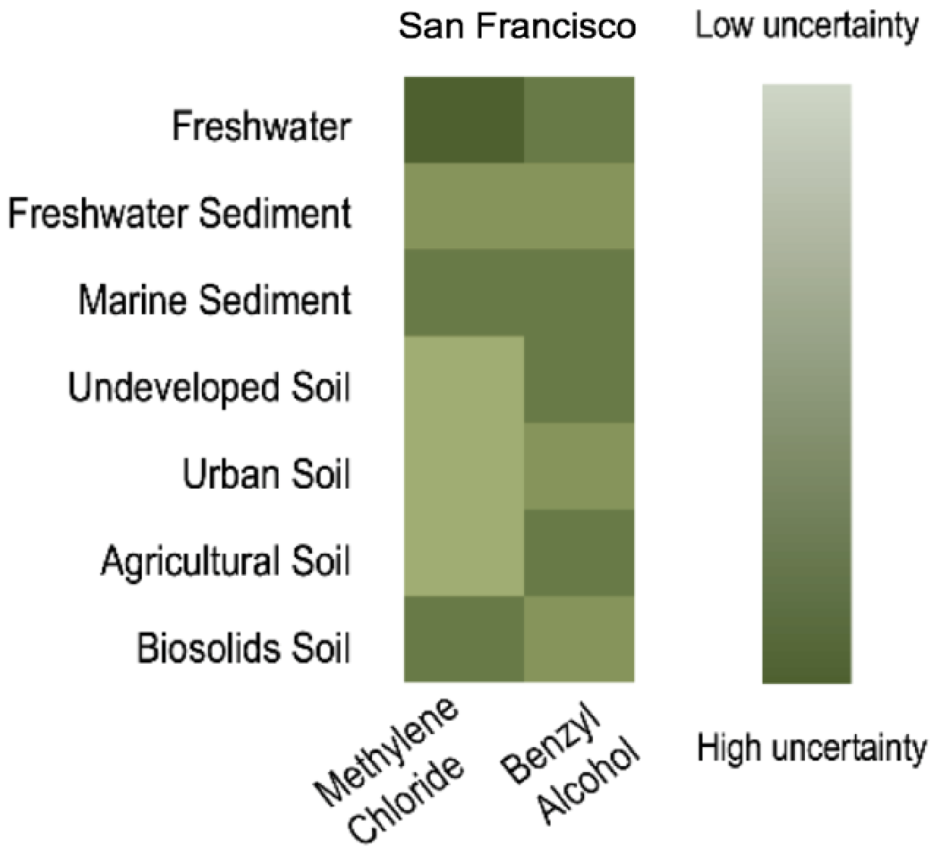
Benzyl Alcohol

Daily intake from ingestion of water	
Deterministic value [kg/(person*d)]	1.33E+04
Probabilistic average [kg/(person*d)]	1.33E+04
Probabilistic median [kg/(person*d)]	1.33E+04
Standard deviation	4.47E-02
Coefficient of variance	3.36E-06
k-value (Slob, 1994)	1.00E+00
k-value (Nunez et al., 2015)	1.00E+00

→ +/-

Examples from CLiCC

Concentrations



→ +/-

Final Step: Presenting the uncertainty in the AA Reports

- Fully describe the uncertainties in the submitted AA report
- Document the uncertainties
  - Key sources of uncertainty and their impacts on the AA results
  - Overall degree of uncertainty that can be placed in the AA results
  - Critical assumptions and their importance to the AA results
  - Unimportant assumptions and why they are considered as unimportant
  - Key conflicting information or key scientific debates involved and how they might impact the AA results

Modified from AA Guide p128

Example 9-4: How Uncertainties in AA Could Be Presented

Uncertainty may be presented in a summary matrix, which lists different sources of uncertainty grouped by types of assessments (i.e., hazard, exposure, and risk characterization) along with the magnitude of uncertainty for each of the sources by using plus/minus signs. An example of an uncertainty summary matrix is shown in the table below.

Example Uncertainty Summary Matrix for Chemical Safety Assessment

	Sources of Uncertainty		Direction & Magnitude of Uncertainty
Hazard traits	Source 1	Model	-
	Source 2	Input parameters	+++
	Source ...	...	...
	Source n	Input parameters	++/--
	Overall effect on hazard estimate E.g.: Mainly affected by overestimation from Source 2, which is uncertainty that may be reduced by ...		
Exposure factors	Source 1	Scenario	++
	Source 2	Model	+
	Source 3	Model	+/-
	Source 4	Input parameters	-
	...	Input parameters	...
	Source m	Input parameters	-
	Overall effect on exposure estimate E.g.: Mainly affected by overestimation from Source 1 and Source 2. Source 1 can be reduced by ...		

Legend: +, ++, +++: low, moderate and high overestimates; -,--, ---: low, moderate and high underestimates

Source: Adapted from European Chemicals Agency (ECHA) Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.19: Uncertainty Analysis. November 2012.

From AA Guide p131

Summary of Uncertainty Analysis

- Follow a structured approach to gather information
- Address two primary categories of data gaps – process-specific and chemical-specific data gaps in AA
- Need to fully consider uncertainties before making a decision
- Document the data in information used – either measured, referenced, or modeled

Modified from AA Guide p128

HANDS-ON EXAMPLES: APPLICATION OF UNCERTAINTY ANALYSIS TOOLS TO SAMPLE SUBSTANCES

Dr. Sangwon Suh (Aug 10th, 1:45pm-2:30pm)

Go to Excel Exercise

QUESTION & ANSWER SESSION